

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.69e-01 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.06e-01

Confidence level: 5.25e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>4-Methylbenzenesulfonic acid</div> <div>Measured: 3.60</div> <div>Predicted: 2.37</div>	<div>Image not found</div> <div>Methylarsonic acid</div> <div>Measured: 1.83</div> <div>Predicted: N/A</div>	<div>Image not found</div> <div>Monosodium methanearsonate</div> <div>Measured: 3.58</div> <div>Predicted: N/A</div>
<div>Image not found</div> <div>Fluopropanate-sodium</div> <div>Measured: 1.31e-01</div> <div>Predicted: 4.65e-01</div>		